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A Lambert W function solution for estimating sustainable injection rates for storage of CO₂ in brine aquifers

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Abstract

It is often of interest to estimate the maximum possible CO₂ injection rate for a given maximum pressure buildup and injection duration scenario. Analytical solutions exist to estimate pressure buildup due to constant rate injection for a specified duration. In this article, it is shown that such solutions can be rearranged for injection rate by virtue of the Lambert W function. It is also shown that the Lambert W function argument is sufficiently small such that a simple asymptotic approximation of the Lambert W function is sufficient in this context.

Key words: CO₂ injection, Geologic carbon sequestration, Pressure buildup, Lambert W function

1. Introduction

In the context of geological carbon sequestration, it is often of interest to estimate the maximum possible CO₂ injection rate for a given maximum pressure buildup and injection duration scenario (e.g. Mathias et al., 2009a, 2013; Ehlig-Economides and Economides, 2010; Okwen et al., 2011a). Much development has been made concerning formulation of analytical solutions to estimate pressure buildup as a consequence of constant rate CO₂ injection (Burton et al., 2008; Vilarrasa et al., 2010; Mathias et al., 2009b, 2011a,b; Okwen et al., 2011b). Although for single phase flow Darcy law problems it is straightforward to rearrange analytical solutions for pressure buildup to solve for injection rate (consider Theis, 1935), for two-phase flow problems (such as CO₂ injection into a brine aquifer), pressure is not a linear function of injection rate. Therefore a simple rearrangement is not possible. More recently, Mathias et al. (2013) used the pressure buildup equation of Mathias et al. (2011b) in conjunction with an iterative approach to obtain a maximum sustainable injection rate for a given pressure and injection duration scenario. In the

current article, the pressure buildup equation of Mathias et al. (2011b) is explicitly rearranged to solve for injection rate by exploitation of an asymptotic expansion of the Lambert W function.

The structure of the article is as follows. A large time approximation for the pressure buildup equation of Mathias et al. (2011b) is briefly described. The problem is then rearranged to yield a Lambert W function solution for injection rate. The appropriate branch of the Lambert W function is determined and the pertinence of an asymptotic expansion in this context is demonstrated. Finally, some comparisons are made with sustainable injection rates predicted using TOUGH2 (Pruess et al., 1999).

2. A large time approximation

Mathias et al. (2011b) derived an analytical solution for one-dimensional radial flow from a well during a constant rate injection of pure CO₂ into a homogenous and isotropic confined brine aquifer originally free of CO₂. Noting that the exponential integral function, $E_1(x)$, can be approximated using $E_1(x) \approx -0.5772 - \ln x + O(x)$, it can be shown that for large times of practical interest (> 1 year), Eq. (57) of Mathias et al. (2011b) reduces to

$$P - P_0 = \frac{\mu_c \alpha (\beta - \epsilon \ln \alpha)}{\mu_b (c_r + c_b)} \quad (1)$$

where P [ML⁻¹T⁻²] and P_0 [ML⁻¹T⁻²] are the current and initial fluid pressures, μ_c [ML⁻¹T⁻¹] is the dynamic viscosity of pure CO₂, μ_b [ML⁻¹T⁻¹] is the dynamic viscosity of brine (free of CO₂), c_r [M⁻¹LT²] is the compressibility of the rock, c_b [M⁻¹LT²] is the compressibility of the brine and α [-] is a dimensionless injection rate defined by

$$\alpha = \frac{M_0 \mu_b (c_r + c_b)}{4\pi H \rho_c k} \quad (2)$$

where M_0 [MT⁻¹] is the mass injection rate of CO₂, H [L] is the formation thickness, ρ_c [ML⁻³] is the density of pure CO₂, k [L²] is permeability and

$$\beta = P_{rpD} - \frac{\ln \zeta}{k_{rs}} - \frac{\mu_b q_{D3} \gamma}{\mu_c} \quad (3)$$

$$\epsilon = \frac{\mu_b q_{D3}}{\mu_c} - \frac{1}{k_{rs}} \quad (4)$$

where P_{rpD} [-] is a dimensionless pressure contribution associated with relative permeability effects, found from Eq. (7) of Mathias et al. (2013), k_{rs} [-] is the permeability reduction factor due to salt precipitation, q_{D3} [-] is a volumetric flow rate reduction factor resulting from CO₂ dissolution in brine, found from Eq. (27) of Mathias et al. (2011b), and ζ is a similarity transform defined by

$$\zeta = \frac{\phi \mu_b (c_r + c_b) r^2}{4kt} \quad (5)$$

where ϕ [-] is porosity, r [L] is radial distance from the origin of the well (set to the well radius when looking at well pressures), t [T] is time, and γ [-] is a term which provides the pressure response of the bulk of the brine aquifer, found from

$$\gamma = \begin{cases} 0.5772, & \zeta_E > 0.5615 \\ \frac{3}{2} - \frac{1}{\zeta_E} - \ln \zeta_E, & \zeta_E < 0.5615 \end{cases} \quad (6)$$

where

$$\zeta_E = \frac{\phi \mu_b (c_r + c_b) r_E^2}{4kt} \quad (7)$$

and r_E [L] is the radial distance from the origin of the injection well to an impermeable outer boundary of the reservoir.

3. Lambert W function solution for injection rate

Eq. (1) can be rearranged to get

$$-\frac{P_D}{\epsilon} \exp\left(-\frac{\beta}{\epsilon}\right) = -\frac{P_D}{\epsilon \alpha} \exp\left(-\frac{P_D}{\epsilon \alpha}\right) \quad (8)$$

where

$$P_D = \frac{\mu_b(c_r + c_b)(P - P_0)}{\mu_c} \quad (9)$$

From Eq. (8), it can be seen that an explicit solution for the dimensionless injection rate, α , can be written as follows

$$\alpha = -\frac{P_D}{\epsilon W\left(-\frac{P_D}{\epsilon} \exp\left(-\frac{\beta}{\epsilon}\right)\right)} \quad (10)$$

where W denotes the Lambert W function whereby $y = W(x)$ satisfies the equation $x = ye^y$ (Coreless et al., 1996).

The Lambert W function has two real branches, referred to as W_0 and W_{-1} , respectively, whereby (Coreless et al., 1996)

$$W(x) = \begin{cases} W_0(x), & W(x) \geq -1 \\ W_{-1}(x), & W(x) < -1 \end{cases} \quad (11)$$

From a practical viewpoint, it can be said that the maximum sustainable injection rate will increase with increasing maximum allowable pressure, i.e.

$$\frac{d\alpha}{dP_D} > 0 \quad (12)$$

Making the substitution

$$x = -\frac{P_D}{\epsilon} \exp\left(-\frac{\beta}{\epsilon}\right) \quad (13)$$

and noting that

$$\frac{dW}{dx} = \frac{W}{x[1 + W(x)]} \quad (14)$$

differentiation of Eq. (10) with respect to P_D leads to

$$\frac{d\alpha}{dP_D} = \frac{-1}{\epsilon[1 + W(x)]} \quad (15)$$

from which it is observed that the constraint given in Eq. (12) is satisfied only when $W(x) < -1$.

Therefore, considering Eq. (11), $W(x) = W_{-1}(x)$. Consequently it can be said that

$$\alpha = -\frac{P_D}{\epsilon W_{-1}\left(-\frac{P_D}{\epsilon} \exp\left(-\frac{\beta}{\epsilon}\right)\right)} \quad (16)$$

4. Evaluating the Lambert W function

The Lambert W function, $W(x)$, can be easily evaluated in MATLAB using the LAMBERTW function (Coreless et al., 1996). However, MATLAB's implementation is computationally quite expensive. Furthermore, the exponential argument in Eq. (13) is generally quite a large negative argument, often leading MATLAB to report zero for the exponential term. Therefore it is worth to consider the asymptotic expansion of $W(x)$ for $x < 0$ and $x \rightarrow 0^-$ (Chapeau-Blondeau and Monir, 2002)

$$W_{-1}(x) = L_1 - L_2 + \frac{L_2}{L_1} + \frac{(-2 + L_2)L_2}{2L_1^2} + \frac{(6 - 9L_2 + 2L_2^2)L_2}{6L_1^3} + O\left(\left\{\frac{L_2}{L_1}\right\}^4\right) \quad (17)$$

where $L_1 = \ln(-x)$ and $L_2 = \ln(-L_1)$.

The exponential term in Eq. (13) is eliminated by substituting Eq. (13) directly into the definition of L_1 to obtain

$$L_1 = \ln\left(\frac{P_D}{\epsilon}\right) - \frac{\beta}{\epsilon} \quad (18)$$

5. Comparison with TOUGH2

Mathias et al. (2013) previously compared the pressure buildup equation, Eq. (57), of Mathias et al. (2011b) (i.e., Eq. (1) in the current article) with well pressures simulated using the numerical simulator, TOUGH2 (Pruess et al., 1999). The simulations involved injecting CO_2 at a constant rate of 15 kg/s for 40 years into three different reservoirs. The three reservoirs were identical

except for the value of exponents, m and n (with m set equal to n), used in the relative permeability functions. The higher the m value, the more non-linear the relative permeability.

In the current article, the pressure data from the TOUGH2 simulations in Fig. 2 of Mathias et al. (2013) is used to demonstrate the effectiveness of Eq. (16) at calculating the optimal injection rate for a given pressure limit. The model parameters used, relevant to Eq. (16), are presented in Table 1. Note that the values of P_{rpD} and q_{D3} for the three relative permeability scenarios were previously calculated (although not reported) by Mathias et al. (2013). These are now presented in Table 2.

From Fig. 2 of Mathias et al. (2013), it is shown that the well pressures in the reservoirs after 2 and 40 years were 14.0 MPa, 14.4 MPa, 15.1 MPa and 16.5 MPa, 16.9 MPa, 17.5 MPa, respectively for the three different relative permeability functions, respectively (as listed in Table 2). The last column of Table 2 contains estimates of sustainable injection rates, along with associated auxiliary variables, for these pressure and duration scenarios (treating the TOUGH2 pressures and times as maximum sustainable pressure and durations of injection, respectively) according to Eq. (16). It can be seen that for the six scenarios studied, estimated injection rate is within 1.3% of the rate determined using TOUGH2. This error is due to the simplifying assumptions made by Mathias et al. (2011b) in the derivation of the pressure buildup equation and numerical error associated with the solvers used within TOUGH2. Note that when pressures calculated using Eq. (57) of Mathias et al. (2011b) are used instead, the error is found to be zero, because Eq. (16) has been mathematically derived directly from Eq. (57).

6. Summary and conclusion

The focus of this article was to provide an explicit means of estimating a maximum sustainable CO₂ injection rate for a given maximum pressure buildup and temperature scenario. For single-phase flow Darcy law problems this is straightforward because injection rate is a linear function of pressure. However, for two-phase flow problems, the relationship between pressure and injection rate becomes non-linear. Nevertheless, it was shown that, for the two-phase flow pressure buildup equation of Mathias et al. (2011b), an explicit solution for injection rate can be derived (i.e., Eq. (16)) by virtue of the Lambert W function. Although the Lambert W function has two real

Table 1: Parameters used for the TOUGH2 comparison.

Parameter	Symbol	Value
Injection rate,	M_0	= 15 kg/s
Well radius,	r_W	= 0.2 m
Radial extent,	r_E	= 20 km
Porosity,	ϕ	= 0.2
Rock compressibility,	c_r	= 4.5×10^{-10} Pa ⁻¹
Initial pressure,	P_0	= 10 MPa
Permeability reduction factor due to salt precipitation,	k_{rs}	= 1
Formation thickness,	H	= 30 m
Permeability,	k	= 100 mD
CO ₂ density,	ρ_c	= 797 kg/m ³
CO ₂ viscosity,	μ_c	= 7.10×10^{-5} Pa s
Brine viscosity,	μ_b	= 9.63×10^{-4} Pa s
Brine compressibility,	c_b	= 3.54×10^{-10} Pa ⁻¹

Table 2: Injection rate estimation based on TOUGH2 pressures.

t (yrs)	m, n	P (MPa)	P_{rpD}	q_{D3}	$\ln \zeta$	ζ_E	γ	β	ϵ	P_D	$\ln(-x)$	$W_{-1}(x)$	α	M_0 (kg/s)
2	1	14.0	5.3	0.955	-22.1	2.45	0.58	20.0	12.0	0.044	-7.3	-9.5	0.000384	14.9
2	2	14.4	13.5	0.971	-22.1	2.45	0.58	28.1	12.2	0.048	-7.8	-10.2	0.000389	15.1
2	3	15.1	31.1	0.970	-22.1	2.45	0.58	45.7	12.2	0.055	-9.1	-11.6	0.000392	15.2
40	1	16.5	5.3	0.955	-25.1	0.12	-4.55	89.4	12.0	0.071	-12.6	-15.3	0.000385	14.9
40	2	16.9	13.5	0.971	-25.1	0.12	-4.55	98.6	12.2	0.075	-13.2	-16.0	0.000386	15.0
40	3	17.5	31.1	0.970	-25.1	0.12	-4.55	116.2	12.2	0.082	-14.6	-17.4	0.000387	15.0

branches, it was further shown that solution to practical problems will always involve the W_{-1} branch. Furthermore, the Lambert function argument is generally likely to be very small, which means that a simple asymptotic approximation for the Lambert W function is sufficient in this context. A comparison of estimated injection rates for six scenarios with those predicted using the TOUGH2 results, previously presented by Mathias et al. (2013), shows the new equation to be an accurate approximation of the complete dynamic problem.

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References

- Burton, M., N. Kumar, and S. L. Bryant (2008), Time-dependent injectivity during CO₂ storage in aquifers, SPE/DOE Improved Oil Recovery Symposium, Tulsa, SPE 113937.

- Chapeau-Blondeau, F., Monir, A. (2002), Numerical evaluation of the Lambert W Function and application to generation of generalized Gaussian noise with exponent $1/2$, *IEEE Trans. Signal Processing*, 50, 2160–2165.
- Corless, R. M., Gonnet, G. H., Hare, D. E. G., Jeffrey, D. J., Knuth, D. E. (1996), On the Lambert W function, *Adv. Comput. Math.*, 5, 329–359.
- Ehlig-Economides, C. A., and M. J. Economides (2010) Sequestering carbon dioxide in a closed underground volume, *J. Pet. Sci. Eng.*, 70, 123–130, doi:10.1016/j.petrol.2009.11.002.
- Mathias S. A., P. E. Hardisty, M. R. Trudell, and R. W. Zimmerman (2009a), Screening and selection of sites for CO₂ sequestration based on pressure buildup, *Int. J. Greenhouse Gas Control*, 3, 577–585, doi:10.1016/j.ijggc.2009.05.002.
- Mathias S. A., P. E. Hardisty, M. R. Trudell, and R. W. Zimmerman (2009b), Approximate solutions for pressure buildup during CO₂ injection in brine aquifers, *Transp. Porous Media*, 79, 265–284, doi:10.1007/s11242-008-9316-7.
- Mathias S. A., G. J. Gonzalez Martinez de Miguel, K. E. Thatcher, and R. W. Zimmerman (2011a), Pressure buildup during CO₂ injection into a closed brine aquifer, *Transp. Porous Media*, In Press, doi:10.1007/s11242-011-9776-z.
- Mathias S. A., J. G. Gluyas, G. J. Gonzalez Martinez de Miguel, S. A. Hosseini (2011b), Role of partial miscibility on pressure buildup due to injection of CO₂ into closed and open brine aquifers, *Water Resour. Res.* 47, W12525, doi:10.1029/2011WR011051.
- Mathias S. A., J. G. Gluyas, G. J. Gonzalez Martinez de Miguel, S. L. Bryant, D. Wilson (2013), On relative permeability data uncertainty and CO₂ injectivity estimation for brine aquifers, *Int. J. Greenhouse Gas Control* 12, 200–212, doi:10.1016/j.ijggc.2012.09.017.
- Okwen, R. T., M. T. Stewart, J. A. Cunningham (2011a), Temporal variations in near-wellbore pressures during CO₂ injection in saline aquifers, *Int. J. Greenhouse Gas Control*, In Press, doi:10.1016/j.ijggc.2011.07.011.
- Okwen, R. T., M. T. Stewart, J. A. Cunningham (2011b), Analytical model for screening potential CO₂ repositories, *Computational Geosciences*, 15, 755–770, doi:10.1007/s10596-011-9246-2.
- Pruess, K., C. M. Oldenburg, and G. Moridis (1999), TOUGH2 users guide, version 2.0. Report LBNL-43134, Lawrence Berkeley National Laboratory, Berkeley, CA, USA.
- Theis CV (1935) The relationship between the lowering of the piezometric surface and the rate and duration of discharge of a well using ground water storage. *Trans Amer Geophys Union* 16:519–524
- Vilarrasa V., Bolster D., Dentz M., Olivella S., Carrera J. (2010) Effects of CO₂ Compressibility on CO₂ Storage in Deep Saline Aquifers. *Trans Porous Media* 85,619–639, doi:10.1007/s11242-010-9582-z.